2,6-Dichlorobenzyl alcohol, n-propyl ether

Inchi: InChI=1S/C10H12Cl2O/c1-2-6-13-7-8-9(11)4-3-5-10(8)12/h3-5H,2,6-7H2,1H3
InchiKey: OBGSDANJGMRJTG-UHFFFAOYSA-N
Formula: C10H12Cl2O
SMILES: CCCOCc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 219.11

Physical Properties

Property code	Value	Unit	Source
gf	-2.39	kJ/mol	Joback Method
hf	-199.84	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hvap	52.63	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.920		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	1486.00		NIST Webbook
rinpol	1486.00		NIST Webbook
tb	562.12	K	Joback Method
tc	777.56	K	Joback Method
tf	335.99	K	Joback Method
vc	0.604	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.42	J/mol×K	562.12	Joback Method
cpg	391.74	J/mol×K	741.66	Joback Method
cpg	381.78	J/mol×K	705.75	Joback Method
cpg	371.18	J/mol×K	669.84	Joback Method
cpg	359.93	J/mol×K	633.93	Joback Method
cpg	348.02	J/mol×K	598.03	Joback Method
cpg	401.07	J/mol×K	777.56	Joback Method
dvisc	0.0001876	Pa×s	562.12	Joback Method

dvisc	0.0002316	Pa×s	524.43	Joback Method
dvisc	0.0002954	Pa×s	486.74	Joback Method
dvisc	0.0003924	Pa×s	449.06	Joback Method
dvisc	0.0005492	Pa×s	411.37	Joback Method
dvisc	0.0008226	Pa×s	373.68	Joback Method
dvisc	0.0013489	Pa×s	335.99	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378129&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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